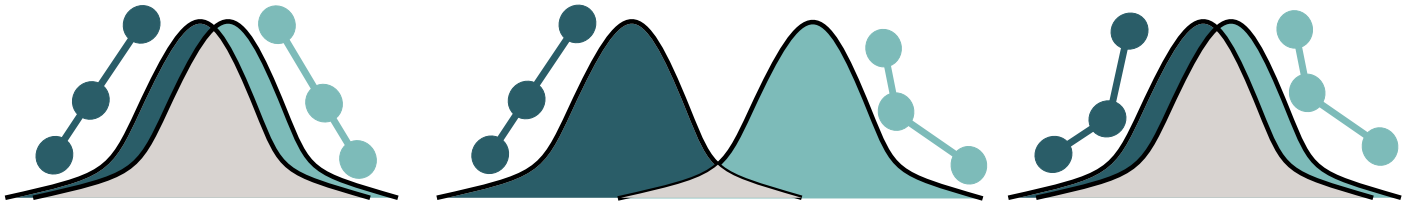
Quantum Fidelity Susceptibility as a tool to characterize shape transitions in molecular bending spectra

Jamil Khalouf-Rivera, Miguel Carvajal, Francisco Pérez-Bernal



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Outline

- Quantum Fidelity Susceptibility (QFS)
- Excited State Quantum Phase Transition (ESQPT)
- The 2D limit of the Vibron Model (2DVM)
- Some real cases
- Effect of the bent-to-linear transition over the QFS
- Effect HCN-HNC isomerization over the QFS

QFS and ESQPT

Ref: W.L. You et al. *Phys. Rev. E*, 76:022101, 2007

Ref: P. Cejnar et al. *J. Phys. A: Math. Theor.*, 54(13):133001, 2021

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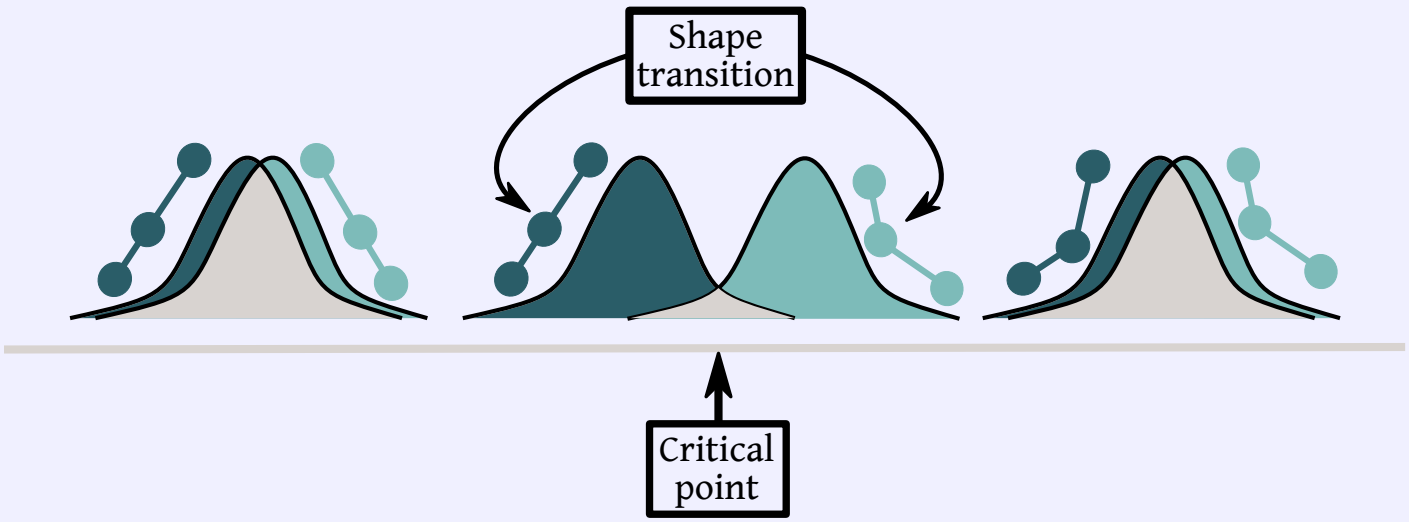

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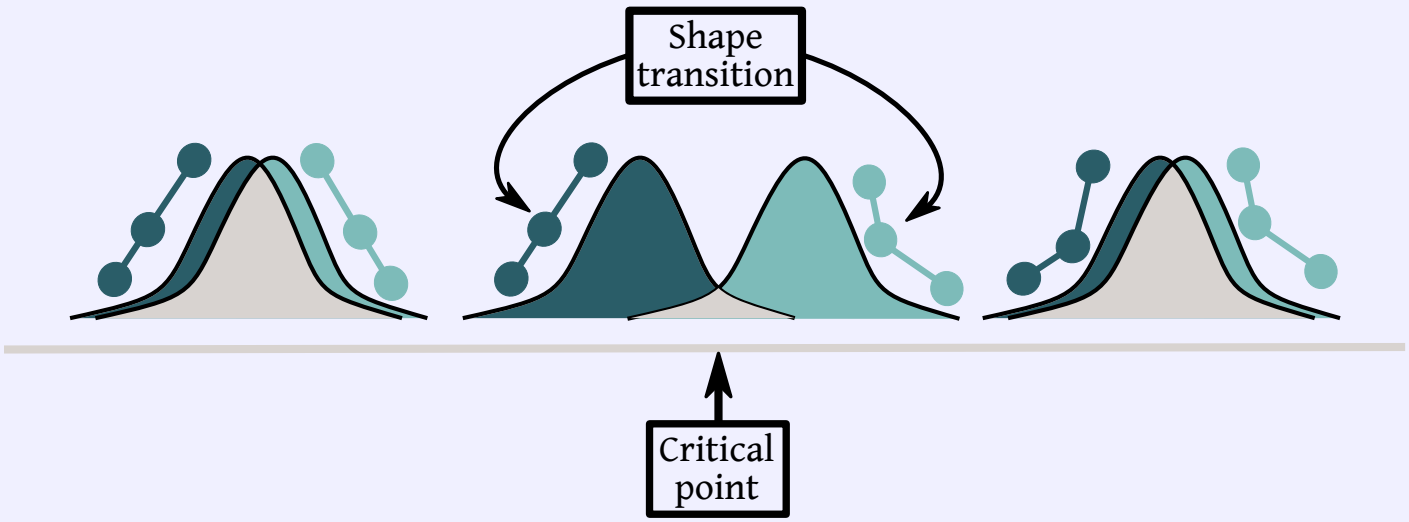

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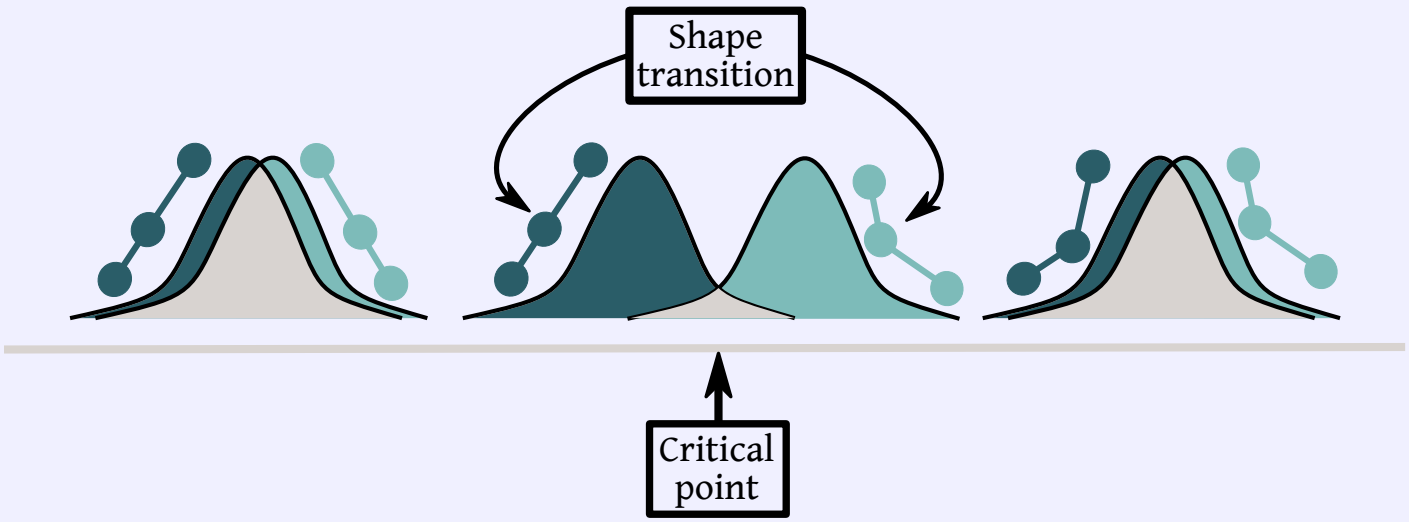

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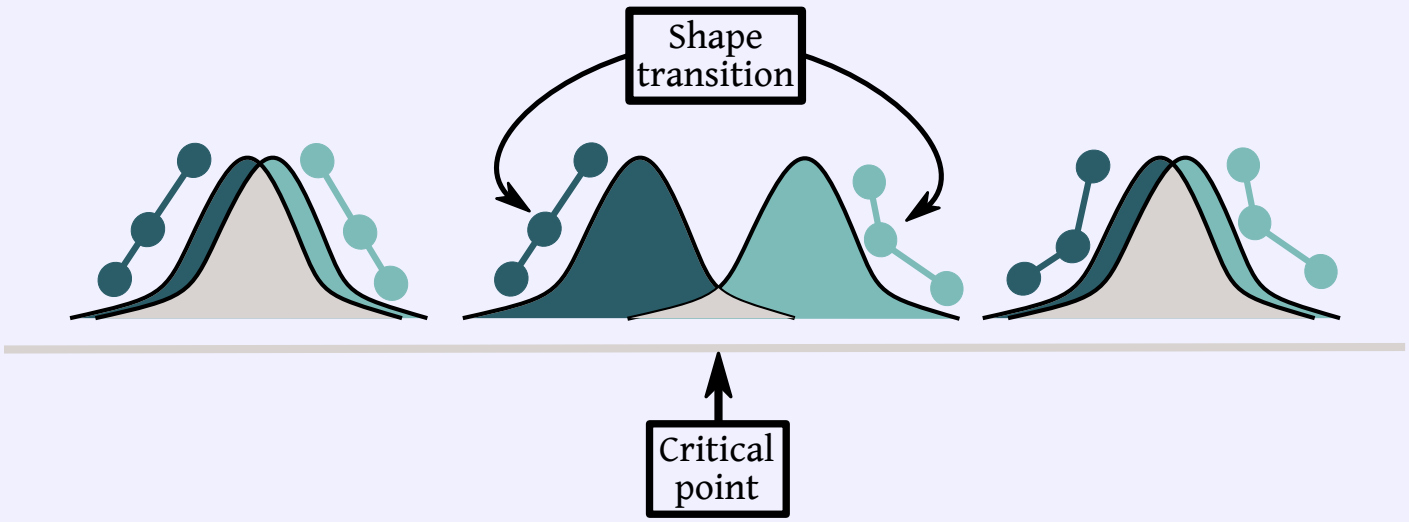

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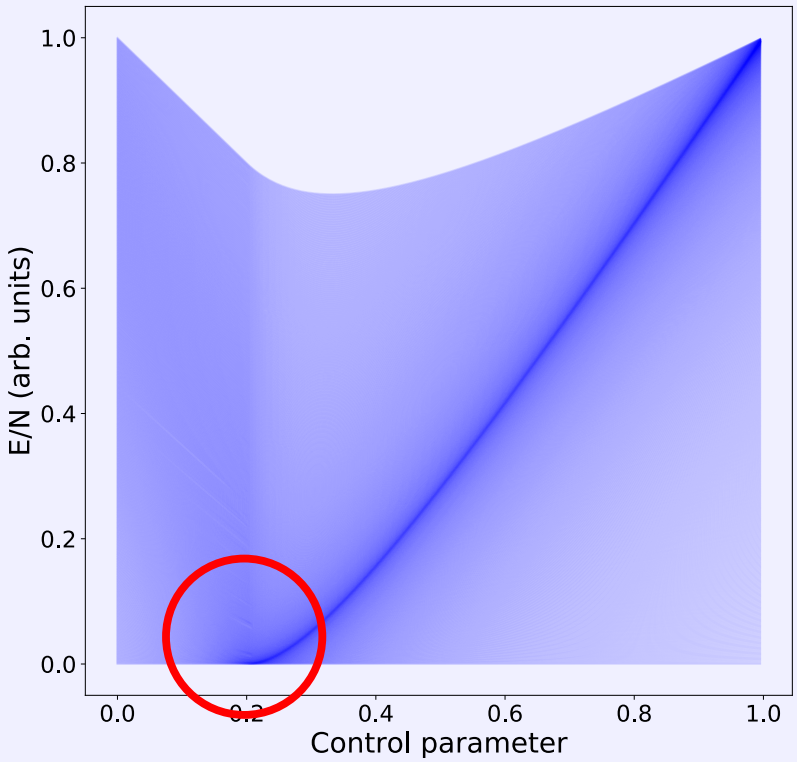

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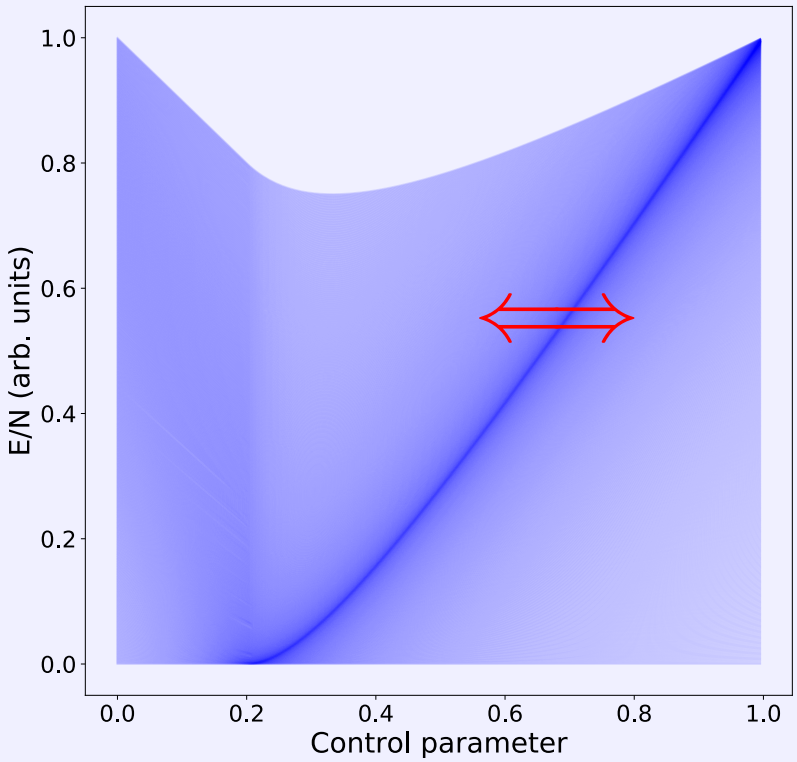

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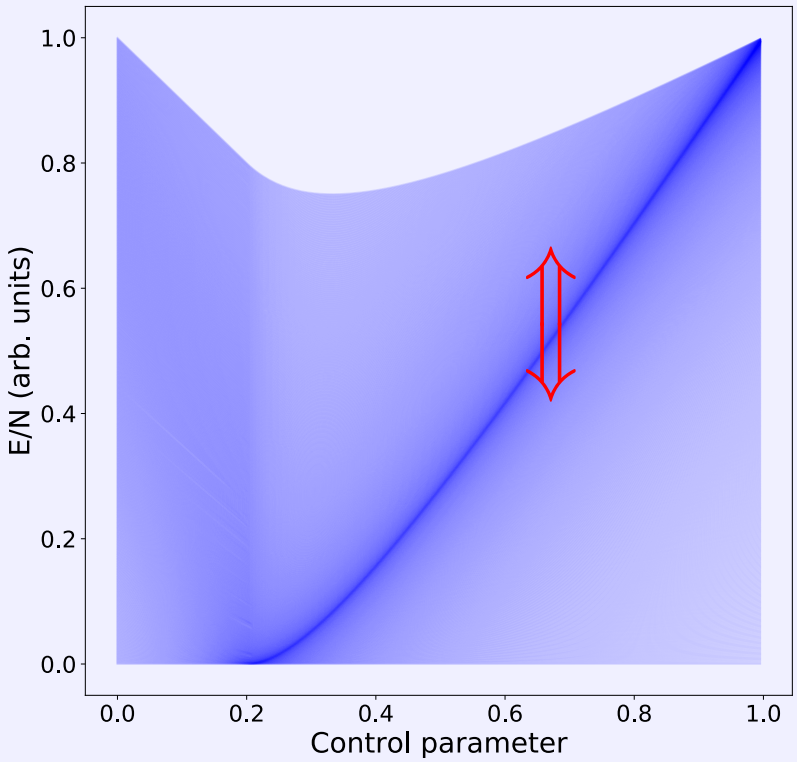

The 2D limit of the vibron model

Ref: F. Iachello et al. *J. Chem. Phys.*, 104(18):6956–6963, 1996

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Bosonic operators

$$\tau_x, \tau_x^\dagger, \tau_y, \tau_y^\dagger, \sigma, \sigma^\dagger$$

Circular bosonic operators

$$\tau_\pm^\dagger = \frac{\mp 1}{\sqrt{2}} \left(\tau_x^\dagger \pm i\tau_y^\dagger\right)$$
$$\tau_\pm = \frac{\mp 1}{\sqrt{2}} \left(\tau_x \mp i\tau_y\right)$$

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$U(3)$ algebra

$$U(3) = \left\langle \tau_i^\dagger \tau_j, \tau_i^\dagger \sigma, \sigma^\dagger \tau_i, \sigma^\dagger \sigma;\ i,j = x,y \right\rangle$$
$$= \left\langle \hat{n}, \hat{n}_s, \hat{\ell}, \hat{Q}_\pm \hat{R}_\pm, \hat{D}_\pm \right\rangle$$

$$\hat{n} = \tau_+^\dagger \tau_+ + \tau_-^\dagger \tau_-$$
$$\hat{\ell} = \tau_+^\dagger \tau_+ - \tau_-^\dagger \tau_-$$

$$\hat{W}^2 = \frac{1}{2}\left(\hat{D}_+\hat{D}_- + \hat{D}_-\hat{D}_+\right) + \hat{\ell}^2$$
$$\hat{D}_\pm = \sqrt{2}\left(\pm\tau_\pm^\dagger \sigma \mp \sigma^\dagger \tau_\mp\right)$$

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$$
\begin{tikzcd}
 & U(2) \\
U(3) \\
[N] \arrow[ur] \arrow[dr] & \hat{n} \arrow[dr] & SO(2) \\
 & SO(3) \arrow[ur] & \hat{\ell} \\
 & \hat{W}^2
\end{tikzcd}
$$

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$$\begin{tikzcd}
 & \begin{matrix} U(2) \\ \hat{n} \end{matrix} \arrow[dr] & \\
\begin{matrix} U(3) \\ [N] \end{matrix} \arrow[ur] \arrow[dr] & & \begin{matrix} SO(2) \\ \hat{\ell} \end{matrix} \\
 & \begin{matrix} SO(3) \\ \hat{W}^2 \end{matrix} \arrow[ur] &
\end{tikzcd}$$

Chain I (linear)

$$\left| \begin{array}{ccccc} U(3) & \supset & U(2) & \supset & SO(2) \\ [N] & & n & & \ell \end{array} \right\rangle \begin{array}{l} n = 0, 1, \ldots, N \\ \ell = \pm n, \pm(n-2), \ldots, \pm 1 \text{ or } 0 \end{array}$$

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$$\begin{tikzcd}[column sep=small] & U(2) \\ & \hat{n} \\ U(3) \arrow[ur] \arrow[dr] & & \\ [N] & & SO(2) \\ & SO(3) \arrow[uur] \arrow[ur] & \\ & \hat{W}^2 & \\ & & \hat{\ell} \end{tikzcd}$$

Chain II (bent)

$$\left| \begin{array}{ccccc} U(3) & \supset & SO(3) & \supset & SO(2) \\ [N] & & \omega & & \ell \end{array} \right\rangle \quad \begin{array}{l} \omega = N, N-2, ...1 \text{ or } 0 \\ \ell = \pm\omega, \pm(\omega-1), ..., 0 \end{array}$$

$$\nu_b = \frac{N-\omega}{2} \qquad \nu_b = \frac{n-|\ell|}{2}$$

Molecules

[1] JKR et al. *J. Quant. Spectrosc. Radiat. Transf.*, 261:107436, 2021
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Extended Hamiltonian Ref. [1]

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\begin{aligned}
\hat{H}_{4b} = & P_{11}\hat{n} + P_{21}\hat{n}^2 + P_{22}\hat{\ell}^2 + P_{23}\hat{W}^2 + \\
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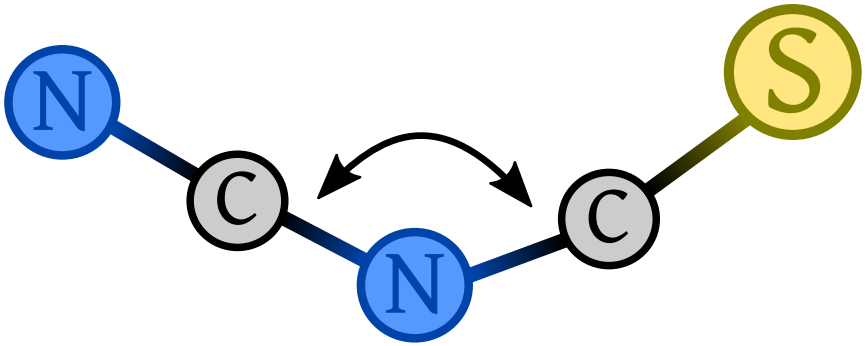

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Bent-to-linear transition

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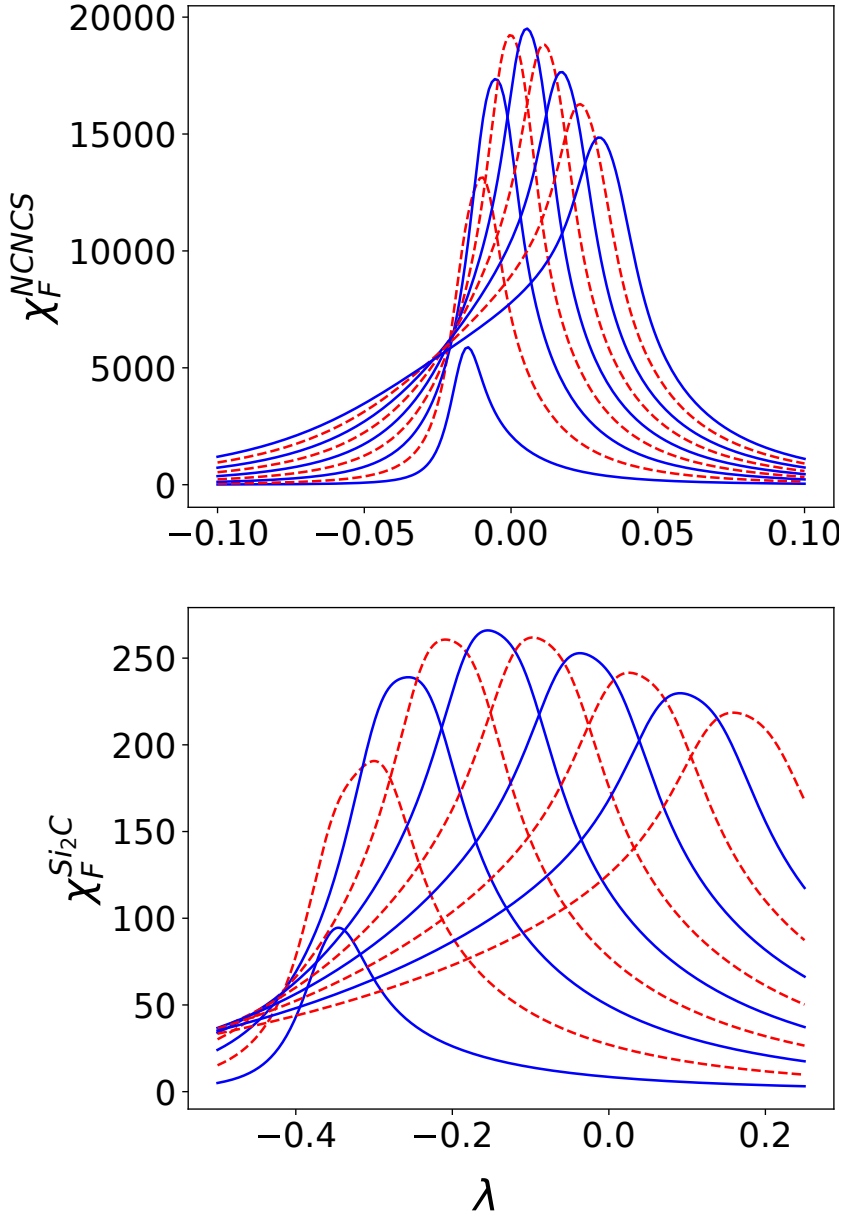

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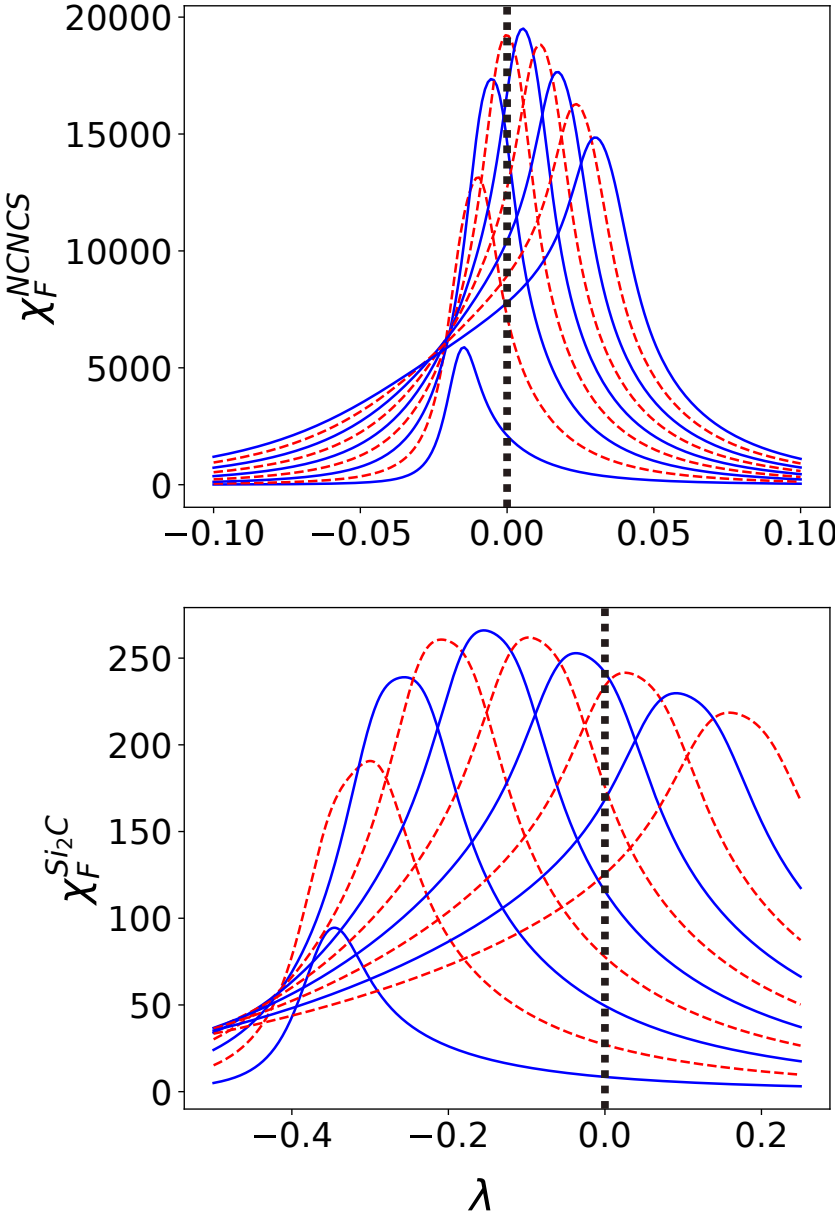

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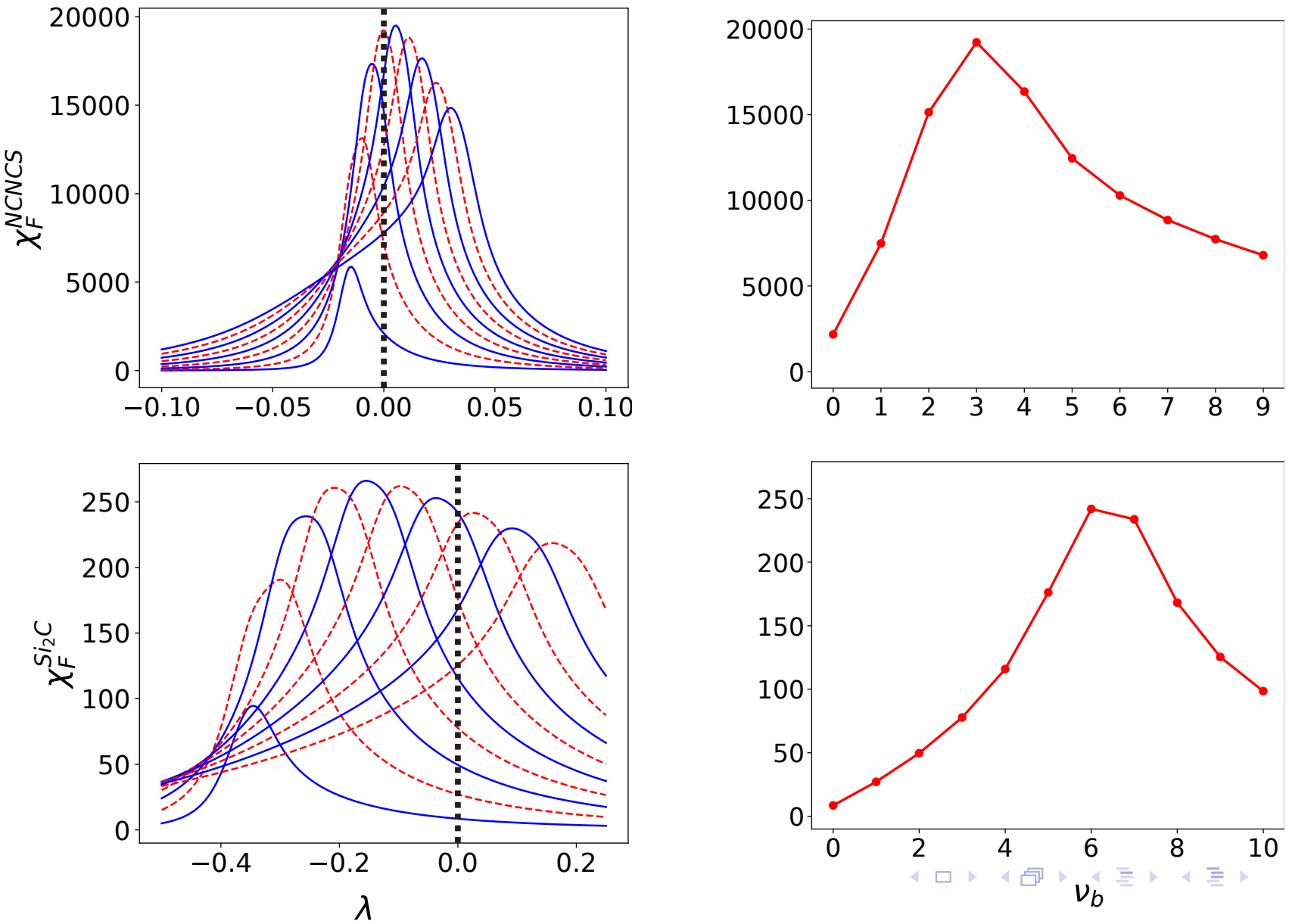

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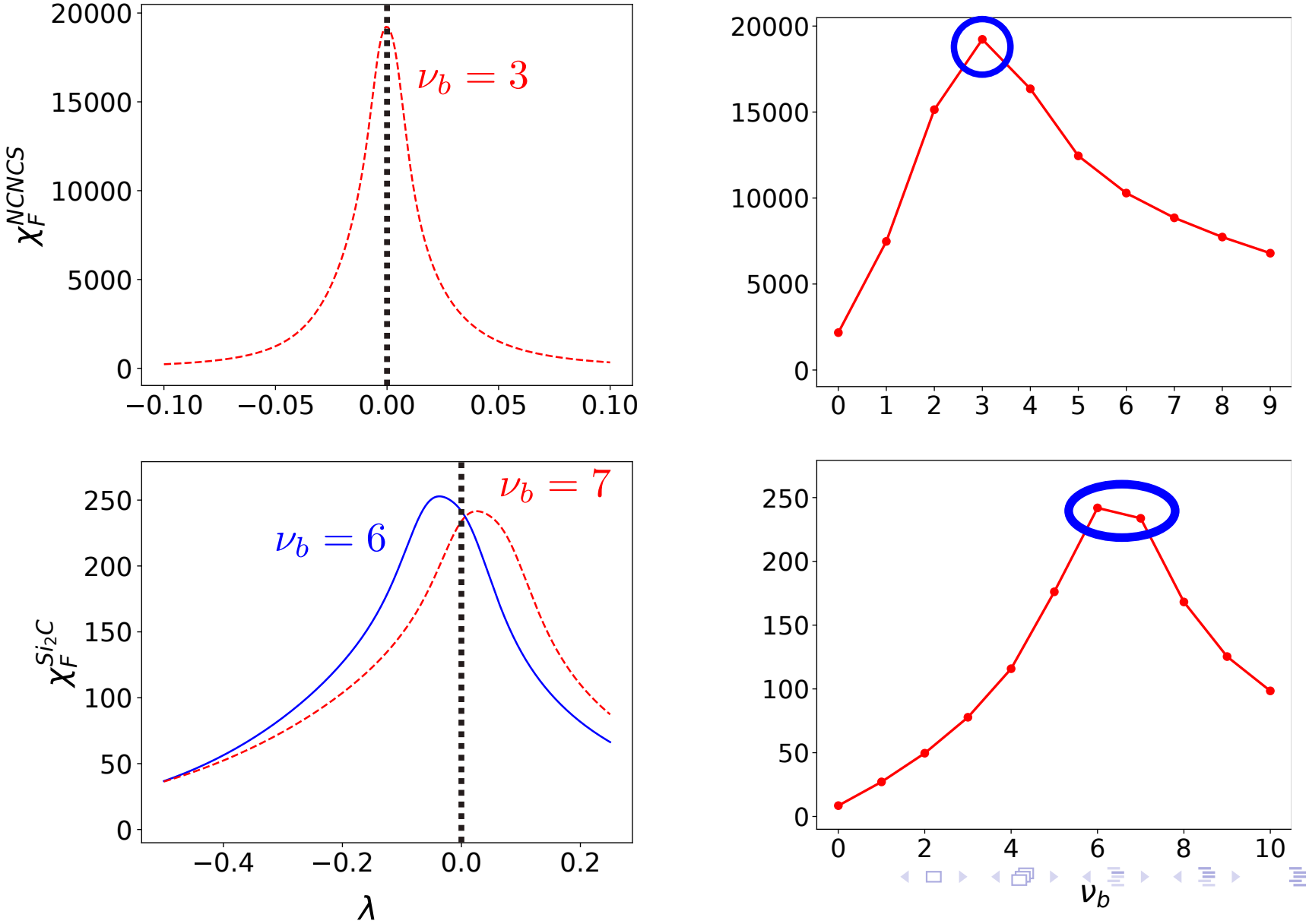
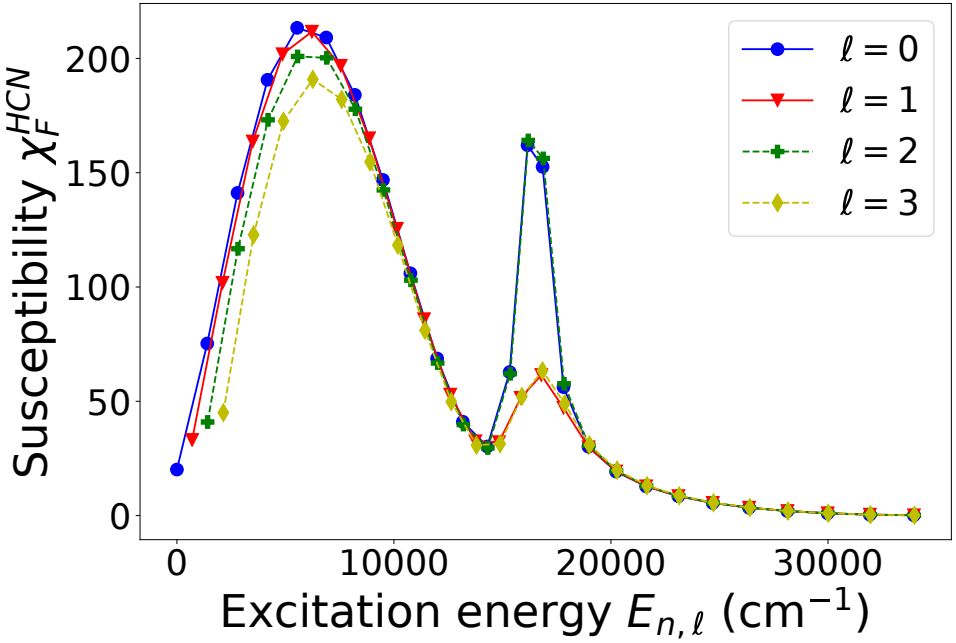
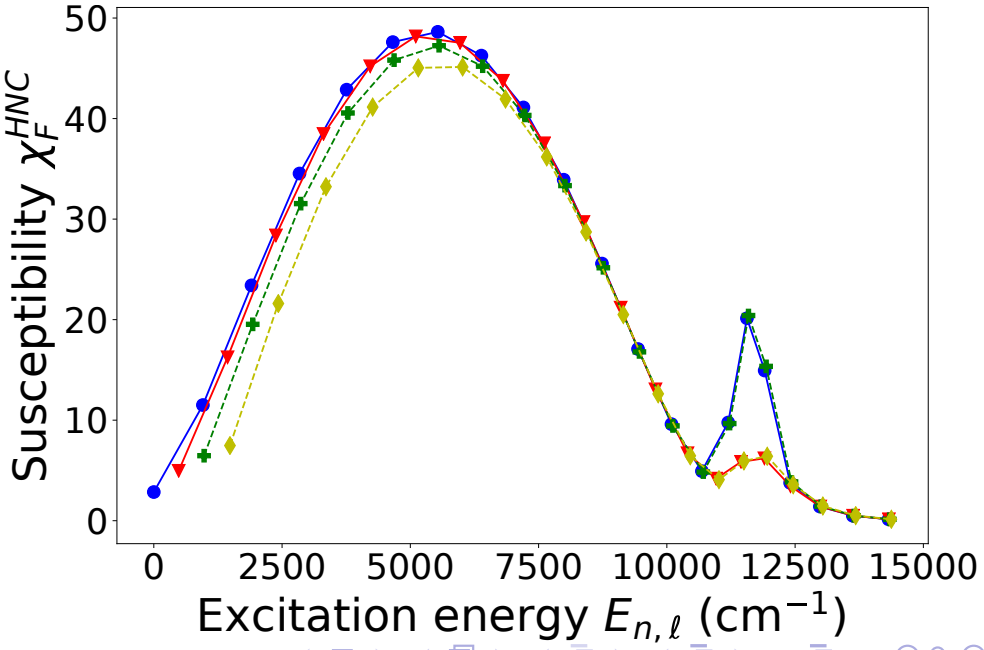


Isomerization

Ref: JKR et al. *J. Phys. Chem. A*, 123(44):9544–9551, 2019

Ref: JKR et al. *Phys. Rev. A*, 105:032215, 2022





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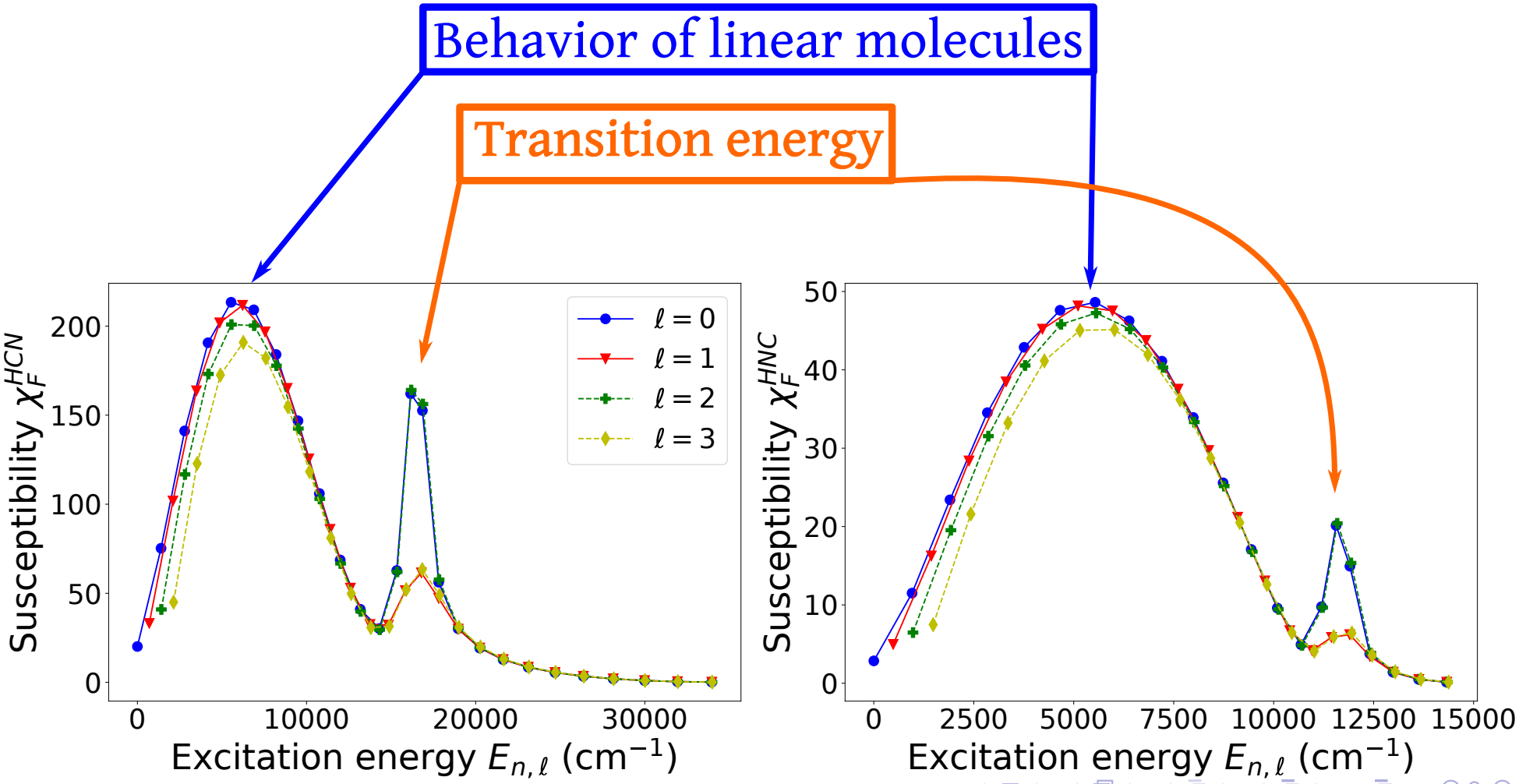
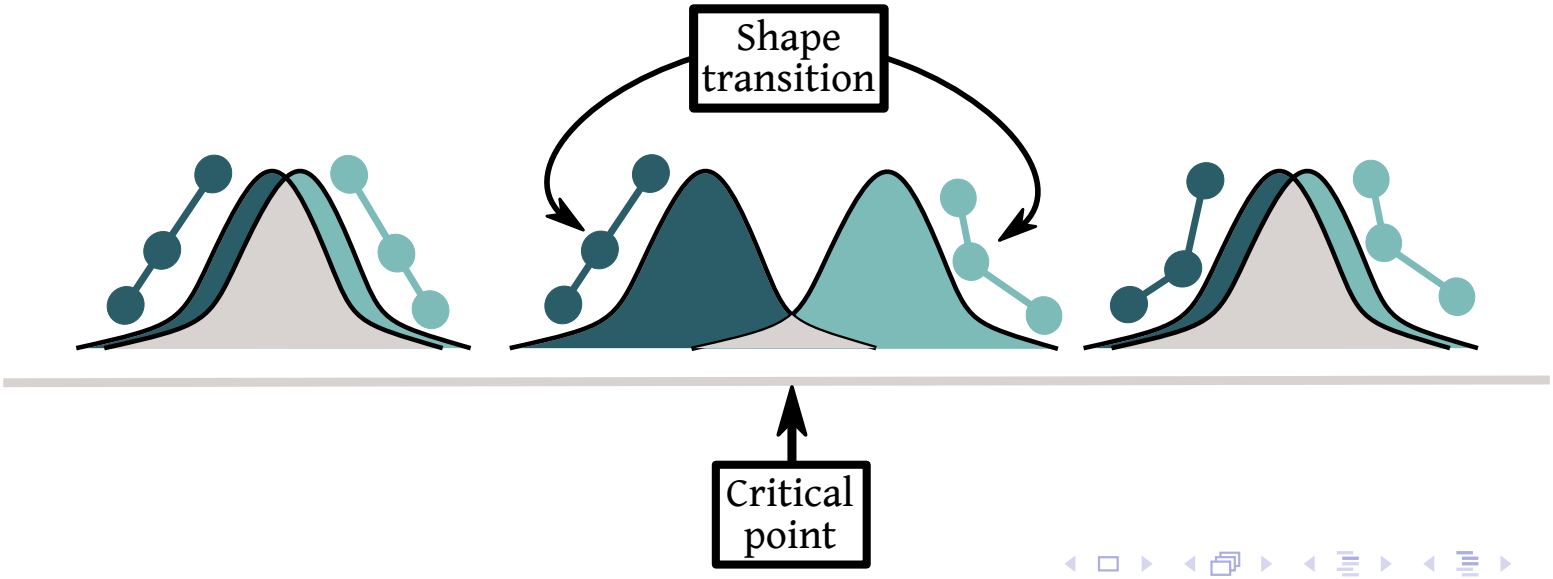


Summary and conclusions

- The QFS is useful beyond the ground state
- Excited spectra can be studied varying both, the control parameter and the energy
- A single control parameter can be defined in real systems
- The QFS is a good marker of shape transitions
  - bent-to-linear transition
  - HCN-HNC isomerization



Thanks for your attention!

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